12:24:05 OCA PAD INITIATION - PROJECT HEADER INFORMATION 05/09/88

Active

Project # G-33-685 Cost share #: Rev #: 0
Center # : Q5455-0A0 Center shr #: OCA file #:
Work type : RES
Contract# 1 S10 RR04192-01 Mod #: Document : GRANT
Prime #: Contract entity: GIT

Subprojects ? : N
Main project #:

Project unit: CHEM Unit code: 02.010.136
Project director(s):
SHOBAUGH J A JR CHEM

Sponsor/division names: DHHS/PHS/NIH / NATL INSTITUTES OF HEALTH
Sponsor/division codes: 08 / 001

Award period: 880411 to 890410 (performance) 890710 (reports)

Sponsor amount	New this change	Total to date
Contract value	96,000.00	96,000.00
Funded	96,000.00	96,000.00
Cost sharing amount		0.00

Does subcontracting plan apply ?: N

Title: COMPUTER AND GRAPHICS FACILITIES FOR MOLECULAR DESIGN

PROJECT ADMINISTRATION DATA

OCA contact: E. Faith Gleason 894-4820

Sponsor technical contact

MARJORIE A. TINGLE, PH.D., DIRECTOR
(301)496-6743
BIOMEDICAL RESEARCH SUPPORT PROGRAM
BLDG 31 RM 5B23, NAT INST OF HEALTH
BETHESDA, MARYLAND 20892

Sponsor issuing office

IVAN HERNANDEZ, OFF GRANT & CONT MGT
(301)496-9840
DIVISION OF RESEARCH RESOURCES
NATIONAL INSTITUTES OF HEALTH
BETHESDA, MARYLAND 20892

Security class (U,C,S,TS) : ONR resident rep. is ACO (Y/N): N
Defense priority rating : supplemental sheet
Equipment title vests with: Sponsor GIT X
PRIOR APPROVALFROM DRR/NIH REQUIRED IF ANY DEVIATION IN APPROVED BASIC EQUIP

Administrative comments -
INITIATION - BIOMEDICAL RESEARCH SUPPORT (BRS) SHARED INSTRUMENTATION GRANT.

12/88

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION

NOTICE OF PROJECT CLOSEOUT

Date 8/8/89

ject No. G-33-635 Center No. Q5455-0A0

ject Director F. L. Suddath, Jr. School/Lab Chemistry

nsor DHHS/PHS/NIH

tract/Grant No. 1 S10 RR04192-01 GTRC ____ GIT XX

me Contract No. N/A

le Computer and Graphics Facilities for Molecular Design

ective Completion Date 4/10/89 (Performance) 7/10/89 (Reports)

seout Actions Required:

_ None
_ Final Invoice or Copy of Last Invoice
_ Final Report of Inventions and/or Subcontracts - Already Submitted.
_ Government Property Inventory & Related Certificate
_ Classified Material Certificate
_ Release and Assignment
_ Other _____

ludes Subproject No(s). _____

project Under Main Project No. _____

tinues Project No. _____ Continued by Project No. _____

tribution:

Project Director
Administrative Network
Accounting
Procurement/GTRI Supply Services
Research Property Management
Research Security Services

X Reports Coordinator (OCA)
___ GTRC
X Project File
2 Contract Support Division (OCA)
___ Other _____

Final Progress Report

Grant No.: 1 S10 RR04192-01

Principal Investigator: Fred L. Suddath, Jr., Georgia Institute of Technology, 225 North Avenue, N. W., Atlanta, Georgia 30332-0400

Funding Period: 4/11/88 - 4/10/89

Name of Instrument: Silicon Graphics Compute Server, Model 4D240S

Total Purchase Cost: $125,000

Total DRR Award: $96,000

Other Sources of Funding: $29,000 - School of Chemistry, Departmental Funds

2. Describe the shared instrumentation purchased, its usage and its impact on the research community, specifically, the NIH funded users.

   The Silicon Graphics Computer Server was purchased for use in the School of Chemistry and Biochemistry at Georgia Tech to support the research efforts of a number of investigators who have funded NIH support. Our original plans were to purchase a VAX 3600 Computer, but the introduction of a Silicon Graphics Compute Server of considerably more power and only slightly more cost was chosen. This facility has provided at least thirty times the computing power to the crystallographic effort at Georgia Tech to the effort of Drs. Powers, May, and Felton in the area of rational drug design and as a general computing facility for scientific data analysis and reduction.

3. Describe the administration, operation, and plans for the maintenance of the instrument.

   The Silicon Graphics Compute Server has been integrated into the School of Chemistry and Biochemistry's computing facility. It is administered by the departmental service committee, which has representatives from each of the divisions of the department. Day-to-day operation is handled by Dr. Don Van Derveer. Dr. Van Derveer is a small molecule crystallographer and is well familiar with the operating system of both the Silicon Graphics, as well as other computing facilities that make up the departmental computer center. Maintenance for the computer is provided from the School of Chemistry and Biochemistry.

4. Describe (in language understanble to the lay public) any research accomplishments resulting from the use of the instrumentation. Explain the developments in terms of their contributions to new knowledge and potential for the improvement of human health. Provide references to publications, if available).

   One area where the Silicon Graphics machine has had a considerable impact, is in the recent structure solution of Human Serum Transferrin. Transferrin is the major iron and

transport proteins in humans and has the unusual ability to solubilize and bind iron +3 The structure of transferrin has been determined by a group in the School of Chemistry and Biochemistry at Georgia Tech and the computing facility was use extensively during the structure solution. A novel method was used for solving the structure and was very computationally intensive. Had these calculations been carried out on existing computers, it would have taken months of additional time solely devoted to the computations. The factor of forty to fifty improvement in computing speed was an enormous help in solving the structure. It is our expectation that a better understanding of the three dimensional structure of transferrin will lead to an improved understanding of the importance of transferrin in binding iron and transporting it from absorption sites in the intestines to storage sites in the liver.

5. None